

Furan  
110-00-9 | DTXSID6020646

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.89            | 0.25 | 0.88           | 0.26 | 0.75       | 0.38 |

Model Results

Predicted value: 5.08 days

Global applicability domain: Inside

Local applicability domain index: 6.81e-01

Confidence level: 8.29e-01

Nearest Neighbors from the Training Set

|  |   |  |
|--|---|--|
| <div>Image not found</div> <div>Hexane, 2,2-dimethyl-</div> <div>Measured: 24.3</div> <div>Predicted: 4.47</div> | <div>Image not found</div> <div>n-Hexane</div> <div>Measured: 157</div> <div>Predicted: 7.45</div>            | <div>Image not found</div> <div>Pentane</div> <div>Measured: 40.7</div> <div>Predicted: 6.52</div> |
| <div>Image not found</div> <div>3-Ethylhexane</div> <div>Measured: 24.3</div> <div>Predicted: 7.04</div>         | <div>Image not found</div> <div>3,3-Dimethylhexane</div> <div>Measured: 40.7</div> <div>Predicted: 4.71</div> |  |